



Ab Initio Molecular Dynamics

By Marx, Dominik / Hutter, Jürg

Condition: New. Publisher/Verlag: Cambridge University Press | Basic Theory and Advanced Methods | The first book on this rapidly growing field for graduate students and researchers, covering a range of methods and applications. | Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes, including chemical reactions, by unifying molecular dynamics and electronic structure theory. This book provides the first coherent presentation of this rapidly growing field, covering a vast range of methods and their applications, from basic theory to advanced methods. This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques in order that readers can understand and assess the merits and drawbacks of commonly used methods. It also discusses the special features of the widely-used Car-Parrinello approach, correcting various misconceptions currently found in research literature. The book also contains pseudo-code and program layout for typical plane wave electronic structure codes, allowing newcomers to the field to understand commonly-used program packages, and enabling developers to improve and add new features in their code. | Part I. Basic Techniques: 1. Setting the stage: why ab initio molecular dynamics?; 2. Getting started: unifying Md and electronic...



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